

Uploading C:\Program Files\Stnexp\Queries\10594710c.str



chain nodes :
6 8 18 19 20 21 23 25
ring nodes :
1 2 3 4 5 13 14 15 16 17
chain bonds :
1-8 5-6 13-23 15-25 16-19 17-18 19-20 20-21
ring bonds :
1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 13-14 13-17 13-23 14-15 15-16 15-25 16-17
17-18 19-20 20-21
exact bonds :
16-19

G1:H,Cb,Hy,Ak

G2:H,M

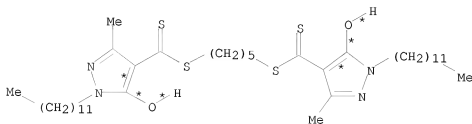
G3:Cb,Hy,Ak

G4:S,SO2

L9 ANSWER 1 OF 3 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 146:242493 CASREACT <<LOGINID::20080928>>
TITLE: Copper(II) complex with the tetradentate ligand
1,5-bis(4-dithiocarboxylate-1-dodecyl-5-hydroxy-3-
methylpyrazolyl)pentane. Liquid-liquid extraction
study
AUTHOR(S): Oliva, Alfonso; Molinari, Aurora; Avila, Carolina;
Flores, Maria Fernanda
CORPORATE SOURCE: Instituto de Quimica, Pontificia Universidad Catolica
de Valparaiso, Chile
SOURCE: Journal of the Chilean Chemical Society (2006), 51(2),
865-867
CODEN: JCCSCB; ISSN: 0717-9324
PUBLISHER: Journal of the Chilean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of the CuDTC (H2DTC = 1,5-bis(4-dithiocarboxylate-1-dodecyl-

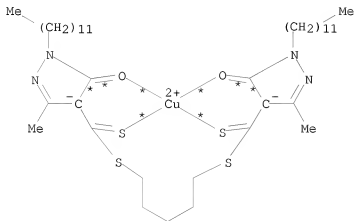
5-hydroxy-3-methylpyrazolyl)pentane) and the solvent extraction behavior of Cu(II) from acid solution (pH 0-5) was studied with the new reagent H2DTC as extractant. The reagent acts as a tetradentate ligand and the extracted species is CuDTC.

RX(1) OF 1 A ==> B



A

(1) →



B

YIELD 96%

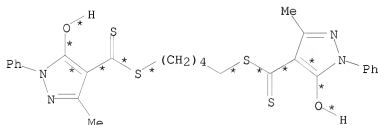
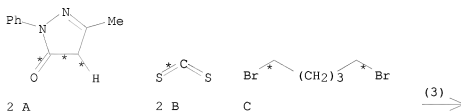
RX(1) RCT A 856015-09-3
 RGT C 142-71-2 Cu(OAc)₂
 PRO B 924890-66-4
 SOL 67-56-1 MeOH, 67-66-3 CHCl₃
 CON overnight, room temperature

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 3 CASREACT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 143:78125 CASREACT <<LOGINID::20080928>>
 TITLE: 1,5-bis(4-dithiocarboxylate-5-hydroxypyrazolyl)pentane
 derivatives of 5-pyrazolones
 AUTHOR(S): Avila, Carolina; Flores, Maria Fernanda; Molinari,

CORPORATE SOURCE: Aurora; Oliva, Alfonso
 Instituto de Química, Pontificia Universidad Católica
 de Valparaíso, Casilla, 4059, Chile
 SOURCE: Journal of Heterocyclic Chemistry (2005), 42(4),
 595-597
 CODEN: JHTCAD; ISSN: 0022-152X
 PUBLISHER: HeteroCorporation
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 3-Methyl-1-phenyl-2-pyrazolin-5-one and 1-dodecyl-3-methyl-2-pyrazolin-5-one react with carbon disulfide and 1,5-dibromopentane in the presence of sodium acetate in DMF or n-butyllithium in THF to afford 1,5-bis(4-dithiocarboxylate-5-hydroxypyrazolyl)pentane derivs.

RX(3) OF 4 2 A + 2 B + C ==> I



I
 YIELD 71%

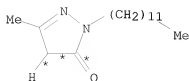
RX(3) RCT A 89-25-8, B 75-15-0

STAGE(1)
 RGT E 127-09-3 AcONa
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 2 hours, 40 deg C
 SUBSTAGE(2) 2 hours, 40 deg C

STAGE(2)
 RCT C 111-24-0
 CON overnight, 40 deg C

PRO I 856015-08-2
 NTE similar results were obtained using BuLi/THF/0C in place of NaOAc/DMF/40C

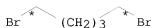
RX(4) OF 4 2 G + 2 B + C ==> J



2 G

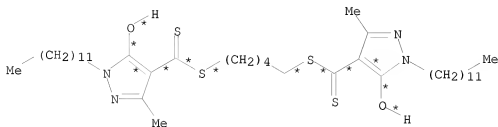


2 B



C

(4) →



J
YIELD 77%

RX(4) RCT G 129803-83-4, B 75-15-0

STAGE(1)

RGT E 127-09-3 AcONa

SOL 68-12-2 DMF

CON SUBSTAGE(1) 2 hours, 40 deg C

SUBSTAGE(2) 2 hours, 40 deg C

STAGE(2)

RCT C 111-24-0

CON overnight, 40 deg C

PRO J 856015-09-3

NTE similar results were obtained using BuLi/THF/0C in place of

NaOAc/DMF/40C

REFERENCE COUNT: 16

THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 3 CASREACT COPYRIGHT 2008 ACS on STN

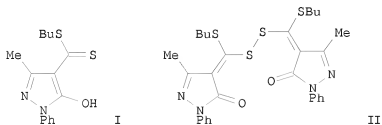
ACCESSION NUMBER: 134:71525 CASREACT <<LOGINID::20080928>>

TITLE: Electrosynthesis of a bis-ketene dithioacetal
disulfide derivative from 1-phenyl-3-methyl-4-(butyl
dithiocarboxylate)-5-pyrazolone using a glassy carbon
electrode

AUTHOR(S): Oliva, Alfonso; Molinari, Aurora; Angulo, Jean;
Schrebler, Ricardo; Gomez, Humberto; Cordova, Ricardo

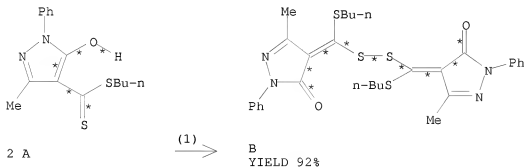
CORPORATE SOURCE: Instituto de Quimica, Universidad Catolica de

SOURCE: Valparaíso, Valparaíso, Chile
 Synthetic Communications (2000), 30(23), 4353-4360
 CODEN: SYNCAV; ISSN: 0039-7911
 PUBLISHER: Marcel Dekker, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The electrooxidn. of pyrazolone dithio ester I was studied in ethanol-water solution, using a glassy carbon electrode surface. The electrochem. and spectroscopic data are in agreement with bis-ketene dithioacetal disulfide II as the only product.

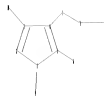
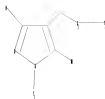
RX(1) OF 1 2 A ==> B



RX(1) RCT A 128202-98-2
 RGT C 7447-41-8 LiCl
 PRO B 314281-72-6
 SOL 64-17-5 EtOH, 7732-18-5 Water
 NTE electrochem.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Uploading C:\Program Files\Stnexp\Queries\10594710e.str



```

chain nodes :
6 7 8 9 10 13
ring nodes :
1 2 3 4 5
chain bonds :
1-9 3-10 4-7 5-6 7-13 8-13
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-9 2-3 3-4 3-10 4-5 5-6 7-13 8-13
exact bonds :
4-7

```

G1:H,Cb,Cy,Hy,Ak

G2:Cb,Cy,Hy,Ak

G3:S,SO2

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
13:CLASS

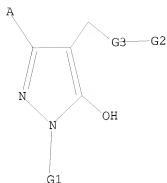
```

L10 STRUCTURE UPLOADED

=> d

L10 HAS NO ANSWERS

L10 STR



G1 H,Cb,Cy,Hy,Ak

G2 Cb,Cy,Hy,Ak

G3 S,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l10 full

FULL SEARCH INITIATED 19:21:54 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 9869 TO ITERATE

100.0% PROCESSED 9869 ITERATIONS

68 ANSWERS

SEARCH TIME: 00.00.01

L11 68 SEA SSS FUL L10

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L11 ANSWER 1 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN

RN 1006311-39-2 REGISTRY

ED Entered STN: 03 Mar 2008

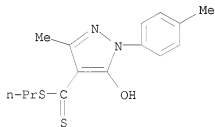
CN 1H-Pyrazole-4-carbodithioic acid, 5-hydroxy-3-methyl-1-(4-methylphenyl)-, propyl ester (CA INDEX NAME)

MF C15 H18 N2 O S2

SR Chemical Library

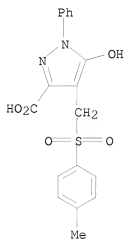
Supplier: Aurora Fine Chemicals

LC STN Files: CHEMCATS



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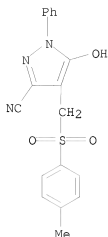
L11 ANSWER 2 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
 RN 866496-21-1 REGISTRY
 ED Entered STN: 01 Nov 2005
 CN 1H-Pyrazole-3-carboxylic acid, 5-hydroxy-4-[[4-methylphenyl)sulfonyl)methyl]-1-phenyl- (CA INDEX NAME)
 MF C18 H16 N2 O5 S
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

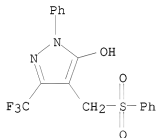
L11 ANSWER 3 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
 RN 866496-20-0 REGISTRY
 ED Entered STN: 01 Nov 2005
 CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-4-[[4-methylphenyl)sulfonyl)methyl]-1-phenyl- (CA INDEX NAME)
 MF C18 H15 N3 O3 S
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L11 ANSWER 4 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 866496-17-5 REGISTRY
ED Entered STN: 01 Nov 2005
CN 1H-Pyrazol-5-ol, 1-phenyl-4-[(phenylsulfonyl)methyl]-3-(trifluoromethyl)-
(CA INDEX NAME)
MF C17 H13 F3 N2 O3 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

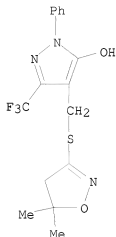


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L11 ANSWER 5 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 866496-16-4 REGISTRY
ED Entered STN: 01 Nov 2005
CN 1H-Pyrazol-5-ol, 4-[[4,5-dihydro-5,5-dimethyl-3-isoxazolyl)thio]methyl]-1-
phenyl-3-(trifluoromethyl)- (CA INDEX NAME)
MF C16 H16 F3 N3 O2 S

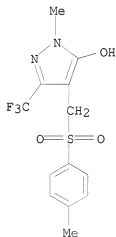
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

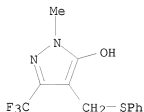
L11 ANSWER 6 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 866496-15-3 REGISTRY
ED Entered STN: 01 Nov 2005
CN 1H-Pyrazol-5-ol, 1-methyl-4-[[4-(trifluoromethyl)phenyl]thiomethyl]-3-
(trifluoromethyl)- (CA INDEX NAME)
MF C13 H13 F3 N2 O3 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



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2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

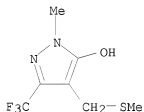
L11 ANSWER 7 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 866496-14-2 REGISTRY
ED Entered STN: 01 Nov 2005
CN 1H-Pyrazol-5-ol, 1-methyl-4-[(phenylthio)methyl]-3-(trifluoromethyl)- (CA
INDEX NAME)
MF C12 H11 F3 N2 O S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L11 ANSWER 8 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 866496-13-1 REGISTRY
ED Entered STN: 01 Nov 2005
CN 1H-Pyrazol-5-ol, 1-methyl-4-[(methylthio)methyl]-3-(trifluoromethyl)- (CA
INDEX NAME)
MF C7 H9 F3 N2 O S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

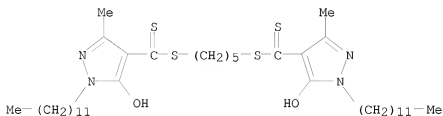


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L11 ANSWER 9 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
RN 856015-09-3 REGISTRY

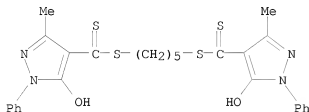
ED Entered STN: 19 Jul 2005
 CN 1H-Pyrazole-4-carbodithioic acid, 1-dodecyl-5-hydroxy-3-methyl-,
 S,S'-1,5-pentanediy l ester (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 1H-Pyrazole-4-carbodithioic acid, 1-dodecyl-5-hydroxy-3-methyl-,
 1,5-pentanediy l ester (9CI)
 MF C39 H68 N4 O2 S4
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT



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2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L11 ANSWER 10 OF 68 REGISTRY COPYRIGHT 2008 ACS on STN
 RN 856015-08-2 REGISTRY
 ED Entered STN: 19 Jul 2005
 CN 1H-Pyrazole-4-carbodithioic acid, 5-hydroxy-3-methyl-1-phenyl-,
 1,5-pentanediy l ester (9CI) (CA INDEX NAME)
 MF C27 H28 N4 O2 S4
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT



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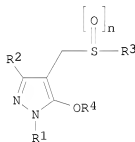
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L13 2 L12

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L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1200395 CAPLUS <<LOGINID::20080928>>
DOCUMENT NUMBER: 143:460143
TITLE: Process for the preparation of 5-difluoromethoxy-4-thiomethylpyrazoles via fluoroalkylation
INVENTOR(S): Uchida, Yukio
PATENT ASSIGNEE(S): Ihara Chemical Industry Co., Ltd., Japan
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005105755	A1	20051110	WO 2005-JP7847	20050425
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
JP 2007246396	A	20070927	JP 2004-132764	20040428
PRIORITY APPLN. INFO.:			JP 2004-132764	A 20040428
OTHER SOURCE(S):	MARPAT 143:460143			
GI				



I

AB A process for the preparation of compound I [R1 = alkyl, (un)substituted aromatic hydrocarbon, (un)substituted heterocycle; R2 = electron withdrawing group; R3 = alkyl, (un)substituted aromatic hydrocarbon, (un)substituted heterocycle; R4 = CHF2; n = 0, 2], characterized by reaction of compds. I [R1, R2, R3, n = same as above; R4 = H] with F2CHX [X = halo] in the presence of sodium hydroxide in dialkyl ketone or alkyl nitrile, was provided. For example, a solution of 3-[(5-hydroxy-1-phenyl-3-

trifluoromethylpyrazol-4-yl)methylthio]-4,5-dihydro-5,5-dimethylisoxazole (33.2 g) and NaOH (12.0 g) in acetonitrile (100 mL) was stirred at room temperature for 1 h. To the resulting mixture was added chlorodifluoromethane (17.3 g) over a period of 4 h, while maintaining the reaction temperature between 5-15 °C. The reaction was stirred for 5 h, followed by work-up and silica-gel purification to afford 3-[(5-difluoromethoxy-1-methyl-3-trifluoromethylpyrazol-4-yl)methylthio]-4,5-dihydro-5,5-dimethylisoxazole (22.6 g).

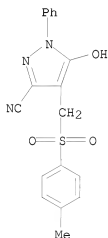
IT 866496-20-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(thiomethylation of pyrazole compds. using formaldehyde)

RN 866496-20-0 CAPLUS

CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-4-[[[(4-methylphenyl)sulfonyl]methyl]-1-phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:1103753 CAPLUS <<LOGINID::20080928>>
 DOCUMENT NUMBER: 143:387027
 TITLE: Process for preparation of 5-hydroxy-4-thiomethylpyrazole derivatives
 Uchida, Yukio
 INVENTOR(S): Ihara Chemical Industry Co., Ltd., Japan
 PATENT ASSIGNEE(S): PCT Int. Appl., 50 pp.
 SOURCE: CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

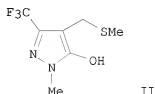
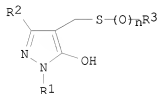
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095352	A1	20051013	WO 2005-JP6806	20050331
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO,				

NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
 RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
 MR, NE, SN, TD, TG

JP 2005289824	A	20051020	JP 2004-102963	20040331
AU 2005228017	A1	20051013	AU 2005-228017	20050331
CA 2560936	A1	20051013	CA 2005-2560936	20050331
CN 1938278	A	20070328	CN 2005-80010635	20050331
EP 1767528	A1	20070328	EP 2005-728918	20050331
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,				
IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR				
BR 2005009353	A	20070911	BR 2005-9353	20050331
KR 2007003964	A	20070105	KR 2006-719480	20060921
IN 2006DN05581	A	20070831	IN 2006-DN5581	20060925
MX 2006PA11130	A	20070125	MX 2006-PA11130	20060928
US 20070185334	A1	20070809	US 2006-594710	20060928
PRIORITY APPLN. INFO.:			JP 2004-102963	A 20040331
			WO 2005-JP6806	W 20050331

OTHER SOURCE(S): MARPAT 143:387027

GI

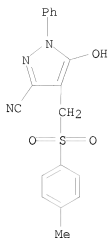


AB This invention pertains to a method for producing pyrazole derivs. I [wherein R1 = H, alkyl, (un)substituted hydrocarbyl, or heterocyclyl; R2 = electron withdrawing group; R3 = alkyl, (un)substituted hydrocarbyl, or heterocyclyl; n = 0 or 2]. For example, 5-hydroxy-1-methyl-3-(trifluoromethyl)pyrazole (preparation given) was reacted with 35% formalin in H2O in the presence of NaOH, followed by the addition of NaSMe to give II (72.7%). This process enables the 5-hydroxy-4-thiomethylpyrazole compds. to be easily produced in high yield under mild conditions through a single step without the necessity of using any special apparatus, expensive catalyst, transition metal, etc. It is friendly to the environment because it generates substantially no harmful wastes derived from a catalyst, etc.

IT 866496-20-0P
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (preparation of 5-hydroxy-4-thiomethylpyrazole derivs.)

RN 866496-20-0 CAPLUS

CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-4-[[4-methylphenyl)sulfonyl)methyl]-1-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
ploading C:\Program Files\Stnexp\Queries\10594710f.str



chain nodes :
6 7 8
ring nodes :
1 2 3 4 5
chain bonds :
1-7 3-8 5-6
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-7 2-3 3-4 3-8 4-5 5-6

G1:H,Cb,Cy,Hy,Ak

G2:Cb,Cy,Hy,Ak

G3:S,S02

Match level :

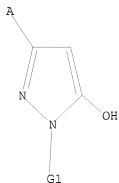
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS

L16 STRUCTURE UPLOADED

=> d

L16 HAS NO ANSWERS

L16 STR



G1 H,Cb,Cy,Hy,Ak

G2 Cb,Cy,Hy,Ak

G3 S,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l16 full

FULL SEARCH INITIATED 19:26:23 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 270331 TO ITERATE

100.0% PROCESSED 270331 ITERATIONS

10523 ANSWERS

SEARCH TIME: 00.00.03

L17 10523 SEA SSS FUL L16

=> s l18 and formaldehyde?

158420 FORMALDEHYDE?

L19 2 L18 AND FORMALDEHYDE?

=> d l19 1-2 ibib abs hitstr

L19 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1200395 CAPLUS <<LOGINID::20080928>>

DOCUMENT NUMBER: 143:460143

TITLE: Process for the preparation of 5-difluoromethoxy-4-thiomethylpyrazoles via fluoroalkylation
Uchida, Yukio

INVENTOR(S): Ihara Chemical Industry Co., Ltd., Japan

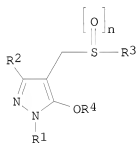
PATENT ASSIGNEE(S): PCT Int. Appl., 27 pp.

SOURCE: CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

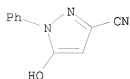
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005105755	A1	20051110	WO 2005-JP7847	20050425
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JP 2007246396	A	20070927	JP 2004-132764	20040428
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OTHER SOURCE(S):			MARPAT 143:460143	
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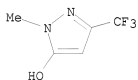
AB A process for the preparation of compound I [R1 = alkyl, (un)substituted aromatic hydrocarbon, (un)substituted heterocycle; R2 = electron withdrawing group; R3 = alkyl, (un)substituted aromatic hydrocarbon, (un)substituted heterocycle; R4 = CHF2; n = 0, 2], characterized by reaction of compds. I [R1, R2, R3, n = same as above; R4 = H] with F2CHX [X = halo] in the presence of sodium hydroxide in dialkyl ketone or alkyl nitrile, was provided. For example, a solution of 3-[(5-hydroxy-1-phenyl-3-trifluoromethylpyrazol-4-yl)methylthio]-4,5-dihydro-5,5-dimethylisoxazole (33.2 g) and NaOH (12.0 g) in acetonitrile (100 mL) was stirred at room temperature for 1 h. To the resulting mixture was added chlorodifluoromethane (17.3 g) over a period of 4 h, while maintaining the reaction temperature between 5-15 °C. The reaction was stirred for 5 h, followed by work-up and silica-gel purification to afford 3-[(5-difluoromethoxy-1-methyl-3-trifluoromethylpyrazol-4-yl)methylthio]-4,5-dihydro-5,5-dimethylisoxazole (22.6 g).

IT 63650-60-2, 3-Cyano-5-hydroxy-1-phenylpyrazole 122431-37-2, 5-Hydroxy-1-methyl-3-trifluoromethylpyrazole
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (thiomethylation of pyrazole compds. using formaldehyde)

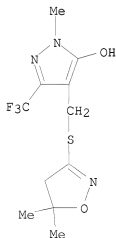
RN 63650-60-2 CAPLUS
 CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-1-phenyl- (CA INDEX NAME)



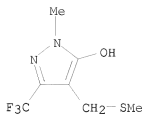
RN 122431-37-2 CAPLUS
 CN 1H-Pyrazol-5-ol, 1-methyl-3-(trifluoromethyl)- (CA INDEX NAME)



IT 447402-29-1P 866496-13-1P 866496-15-3P
 866496-20-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (thiomethylation of pyrazole compds. using formaldehyde)
 RN 447402-29-1 CAPLUS
 CN 1H-Pyrazol-5-ol, 4-[[4,5-dihydro-5,5-dimethyl-3-isoxazolyl)thio]methyl]-1-
 methyl-3-(trifluoromethyl)- (CA INDEX NAME)

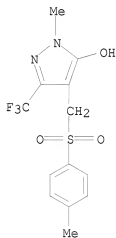


RN 866496-13-1 CAPLUS
 CN 1H-Pyrazol-5-ol, 1-methyl-4-[(methylthio)methyl]-3-(trifluoromethyl)- (CA
 INDEX NAME)



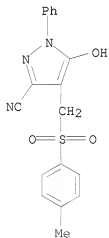
RN 866496-15-3 CAPLUS

CN 1H-Pyrazol-5-ol, 1-methyl-4-[[(4-methylphenyl)sulfonyl]methyl]-3-(trifluoromethyl)- (CA INDEX NAME)



RN 866496-20-0 CAPLUS

CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-4-[[(4-methylphenyl)sulfonyl]methyl]-1-phenyl- (CA INDEX NAME)

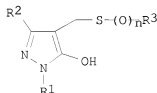


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

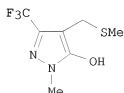
L19 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:1103753 CAPLUS <<LOGINID:20080928>>
 DOCUMENT NUMBER: 143:387027
 TITLE: Process for preparation of 5-hydroxy-4-thiomethylpyrazole derivatives
 INVENTOR(S): Uchida, Yukio
 PATENT ASSIGNEE(S): Ihara Chemical Industry Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 50 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095352	A1	20051013	WO 2005-JP6806	20050331
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JP 2005289824	A	20051020	JP 2004-102963	20040331
AU 2005228017	A1	20051013	AU 2005-228017	20050331
CA 2560936	A1	20051013	CA 2005-2560936	20050331
CN 1938278	A	20070328	CN 2005-80010635	20050331
EP 1767528	A1	20070328	EP 2005-728918	20050331
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR				
BR 2005009353	A	20070911	BR 2005-9353	20050331
KR 2007003964	A	20070105	KR 2006-719480	20060921
IN 2006DN05581	A	20070831	IN 2006-DN5581	20060925
MX 2006PA11130	A	20070125	MX 2006-PA11130	20060928
US 20070185334	A1	20070809	US 2006-594710	20060928
PRIORITY APPLN. INFO.:			JP 2004-102963	A 20040331
			WO 2005-JP6806	W 20050331

OTHER SOURCE(S): MARPAT 143:387027
 GI



I



II

AB This invention pertains to a method for producing pyrazole derivs. I

[wherein R1 = H, alkyl, (un)substituted hydrocarbyl, or heterocyclyl; R2 = electron withdrawing group; R3 = alkyl, (un)substituted hydrocarbyl, or heterocyclyl; n = 0 or 2]. For example, 5-hydroxy-1-methyl-3-(trifluoromethyl)pyrazole (preparation given) was reacted with 35% formalin in H2O in the presence of NaOH, followed by the addition of NaSMc to give II (72.7%). This process enables the 5-hydroxy-4-thiomethylpyrazole compds. to be easily produced in high yield under mild conditions through a single step without the necessity of using any special apparatus, expensive catalyst, transition metal, etc. It is friendly to the environment because it generates substantially no harmful wastes derived from a catalyst, etc.

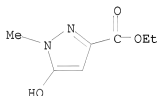
IT 51986-17-5P 63650-60-2P 96145-98-1P

122431-37-2P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of 5-hydroxy-4-thiomethylpyrazole derivs.)

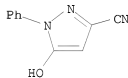
RN 51986-17-5 CAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-hydroxy-1-methyl-, ethyl ester (CA INDEX NAME)



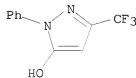
RN 63650-60-2 CAPLUS

CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-1-phenyl- (CA INDEX NAME)



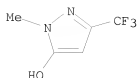
RN 96145-98-1 CAPLUS

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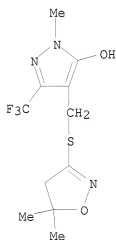


RN 122431-37-2 CAPLUS

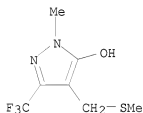
CN 1H-Pyrazol-5-ol, 1-methyl-3-(trifluoromethyl)- (CA INDEX NAME)



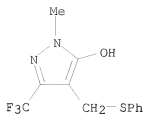
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 866496-15-3P 866496-16-4P 866496-17-5P
 866496-20-0P 866496-21-1P
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
 (Preparation)
 (preparation of 5-hydroxy-4-thiomethylpyrazole derivs.)
 RN 447402-29-1 CAPLUS
 CN 1H-Pyrazol-5-ol, 4-[[{4,5-dihydro-5,5-dimethyl-3-isoxazolyl}thio]methyl]-1-
 methyl-3-(trifluoromethyl)- (CA INDEX NAME)



RN 866496-13-1 CAPLUS
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 INDEX NAME)

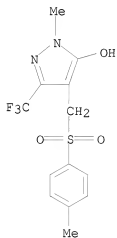


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 INDEX NAME)



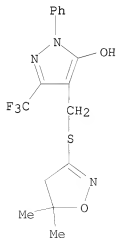
RN 866496-15-3 CAPLUS

CN 1H-Pyrazol-5-ol, 1-methyl-4-[[(4-methylphenyl)sulfonyl]methyl]-3-(trifluoromethyl)- (CA INDEX NAME)



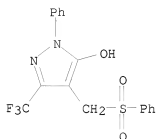
RN 866496-16-4 CAPLUS

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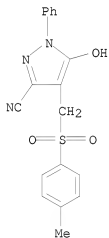
RN 866496-17-5 CAPLUS

CN 1H-Pyrazol-5-ol, 1-phenyl-4-[(phenylsulfonyl)methyl]-3-(trifluoromethyl)-
(CA INDEX NAME)



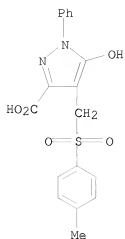
RN 866496-20-0 CAPLUS

CN 1H-Pyrazole-3-carbonitrile, 5-hydroxy-4-[[4-(4-methylphenyl)sulfonyl]methyl]-
1-phenyl- (CA INDEX NAME)



RN 866496-21-1 CAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-hydroxy-4-[[4-(4-methylphenyl)sulfonyl]methyl]-1-phenyl- (CA INDEX NAME)



REFERENCE COUNT:

12

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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